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CALCULATIONS OF THE RELATIVE EFFECTIVENESS OF ALANINE FOR NEUTRONS WITH ENERGIES UP TO 17.1 MeV

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Abstract — The relative effectiveness (RE) of alanine has been calculated for neutrons using the RE of alanine for charged particles. The neutrons interact with one or more of the elements (hydrogen, carbon, nitrogen and oxygen) that compose the alanine. These interactions produce spectra of secondary charged particles consisting of ions of H, D, He, Be, B, C, N, and O. From a combination of the calculated secondary charged particle spectra generated by the slowing down neutrons, and the calculated RE of the ions produced, a RE for the neutrons can be obtained. In addition, lineal energy spectra were determined for neutrons with energies up to 17.1 MeV interacting with alanine. An analytical code was used to calculate these spectra for a 1 μm diameter alanine cell surrounded by an alanine medium. For comparison, similar calculations were made for muscle tissue. Finally, the calculated differential RE was folded with dose distributions to obtain RE-weighted distributions for alanine.

INTRODUCTION

The response of a biological system to various kinds of ionising radiation is described by a concept called relative biological effectiveness (RBE). Similarly, the response of a non-biological system, such as a physical or chemical system, is described by a concept called relative effectiveness (RE). Like RBE, RE can be expressed as a function of linear energy transfer (LET).

The RE of high LET radiation is defined as the ratio of doses from the low and high LET radiations (in this work the low LET radiation is ^{60}Co) that produces the same radiation response under identical target conditions. Unlike most biological systems, physical and chemical systems generally display a decrease in RE with increasing LET and have RE values equal to or less than unity.

Values of RE for alanine exposed to various charged particles have been predicted from model calculations and measured[1,2] using the electron spin resonance technique. This technique can be used since radiation-induced stable free radicals are produced in alanine. RE can be calculated over a wide range of LET and particle parameters, and calculated predictions based on the track structure theory of heavy charged particles[3] show agreement with measured data.

Alanine is a particularly interesting material for use as a detector for radiation dosimetry as it has linearity of response over a wide range of dose, good time stability of the induced free radicals, availability of a non-destructive read-out technique and accuracy and repeatability of measurements. Alanine dosimetry is an attractive alternative to the ferrous sulphate, or Fricke, system of dosimetry. In addition, the chemical composition of alanine $(CH_3\text{-}CH(NH_2)\text{-}COOH)$ is quite close to that of tissue, making the amino acid particularly suitable for neutron dosimetry.

OBJECTIVES

Very little information is available concerning the RE of alanine exposed to neutron radiations. When material is irradiated by neutrons, the ionising radiation produced is principally charged particles. Thus it is possible to calculate the neutron RE of alanine if the initial energy spectra of charged particles caused by neutrons are known, and if the RE of each charged particle is known at each energy.

The first objective of this study is to calculate the RE for alanine irradiated with neutrons having energies between 0.1 MeV and 17.1 MeV. The second objective is to calculate the dose distribution for alanine as a function of lineal energy and compare the result with that of tissue. The third
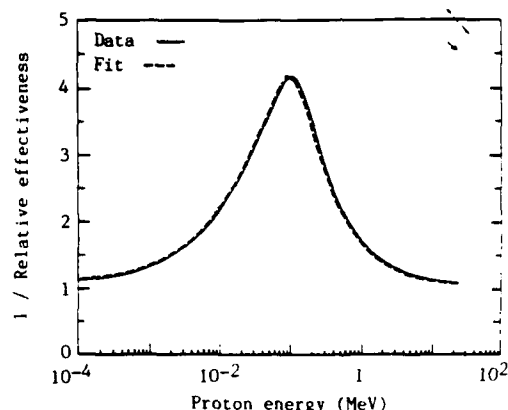
Figure 1. Inverse of the RE of alanine irradiated with protons. These data show the response for completely stopped particles that started with an initial energy given on the abscissa. The solid line is based on calculated and measured data; the dashed line is a modified hyperbolic function fit. A similar hyperbolic function fit was obtained for each of the different charged particles produced by the neutrons.
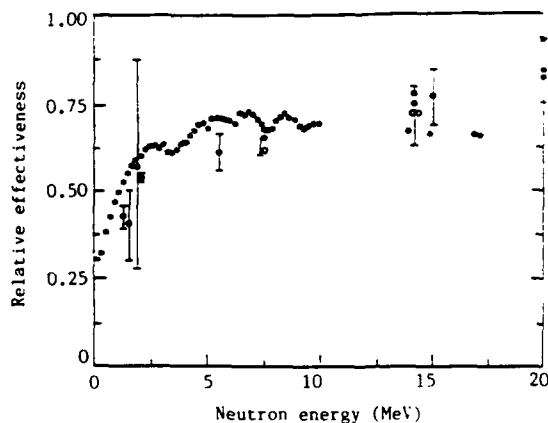

Figure 2. RE for alanine at different neutron energies. The asterisks are the results of our calculations. The solid circles are experimental data and the open circles are calculated data; these data were obtained from the literature on alanine.

objective is to fold the calculated RE with its dose distribution and obtain a RE-weighted dose distribution for alanine.

RELATIVE EFFECTIVENESS

Figure 1 shows the inverse of the RE of alanine exposed to protons. These data show the response for completely stopped particles that started with an initial energy as given on the abscissa. The solid line shows data based on both measurements and

calculations. The dashed line is a fit to these data using a modified hyperbolic function. For each charged particle a similar function with different constants was determined. These functions were then folded with the initial energy spectra of charged particles created by monoenergetic neutrons of a given energy. The RE for alanine was then determined at several neutron energies.

RE is calculated according to

$$
RE = \frac{\sum\limits_{i=1}^{i=K} \int_{0}^{E_{max}} n_i(E) \cdot E \cdot RE_i(E) \cdot dE}{\sum\limits_{i=1}^{i=K} \int_{0}^{E_{max}} n_i(E) \cdot E \cdot dE}
$$

where $n_i(E)$ is the initial energy distribution of the i-th charged particle, and $RE_i(E)$ is RE as a function of energy for the same particle.

Figure 2 shows the RE for alanine calculated by combining the initial energy spectra of charged particles with their RE. Each of our calculated data points is shown as an asterisk over the neutron energy range between 0.1 MeV and 17.1 MeV. The oscillations of the data points are due to experimental variations in the nuclear cross section data used to calculate the initial spectra of heavy ions. Results of the measurements for the RE, as found in the literature[4], are shown as solid points with indicated error bars. Results of three other calculations are shown as open circles at 7.5 MeV and 14.0 MeV[4].

Relative to the measured data, our calculated data give a higher RE below 6 MeV and a lower RE above 13 MeV. Our calculated data consider neutrons that are nearly monoenergetic; the neutron energy bin width is only 200 keV wide. This contrasts with the measured data in which the neutrons are polyenergetic, with neutron energies in some cases ranging over many MeV of energy. The measurements must also extract the large RE contribution due to photons in the neutron beams.

The primary input for our calculations is the ENDF/B-V nuclear data file[5] of the National Nuclear Data Center at Brookhaven; a more recent evaluated data set[6,7] was used for the carbon cross section. The computer program developed at the National Institute of Standards and Technology[8,9] was used for the calculations.

DOSE DISTRIBUTIONS

Figure 3 shows the calculated dose distribution for a 1 μm cavity as a function of lineal energy (y). The radiation source was monoenergetic neutrons at 1.1 MeV. Figure 4 shows the same except the neutron energy was 16.9 MeV. We assumed that the cavity and surrounding wall were made of the same material. Calculations were then made where

material was either tissue or alanine. The curves in Figures 3 and 4 indicate how the dose distribution varies between the two materials. RE values determined in the previous section were not used in these calculations.

The major contribution to the dose at a neutron energy of 1.1 MeV is due to elastically-scattered protons from hydrogen contained in both tissue and alanine. The dose from the protons shows as a broad peak centred near 50 keV.μm^{-1} in Figure 3. The calculated dose is higher for tissue because tissue has 29% more hydrogen. The dose above the proton cut-off at 150 keV.μm^{-1} is due to a small number of heavy-ion recoils. Table 1 gives percentage by weight of the elemental composition for alanine[16] and tissue. The composition of tissue is given by the International Commission on Radiation Units and Measurements (ICRU)[11].

At 16.9 MeV, the broad peak due to the protons shifts down in lineal energy and is centred near 7 keV.μm^{-1} in Figure 4. The shift occurs because the rate of energy loss in the cavity is less for higher energy protons caused by the 16.9 MeV neutrons than for low energy protons caused by the 1.1 MeV neutrons.

Like the calculation at a neutron energy of 1.1 MeV, the dose distribution from the 16.9 MeV neutrons in the lineal energy region of 7 keV.μm^{-1} is greater for tissue than for alanine. However, in the region above 150 keV.μm^{-1}, the reverse holds true: the dose distribution from alanine is greater than that of tissue because the alanine has a larger fraction of carbon and nitrogen compared with tissue. For these elements at this neutron energy, more reaction channels are open for producing alpha particles and heavy ion recoils: these ions contribute a substantial dose in this lineal energy region.
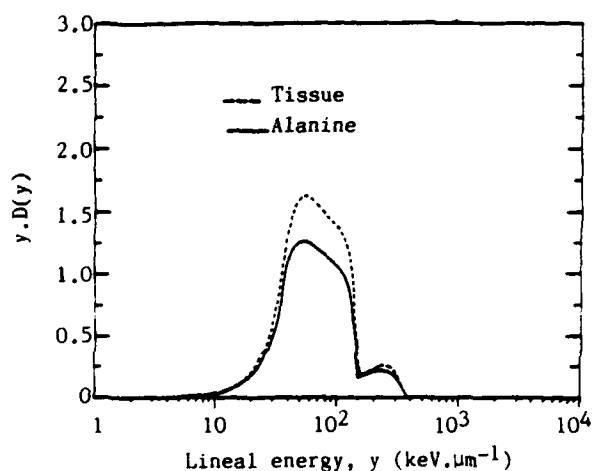

Figure 3. Calculated dose distributions in lineal energy for alanine and tissue at a monoenergetic neutron energy of 1.1 MeV. The solid line is the result for alanine and the dashed line is the result for ICRU tissue. The large peaks are caused by the dose contribution from the protons.
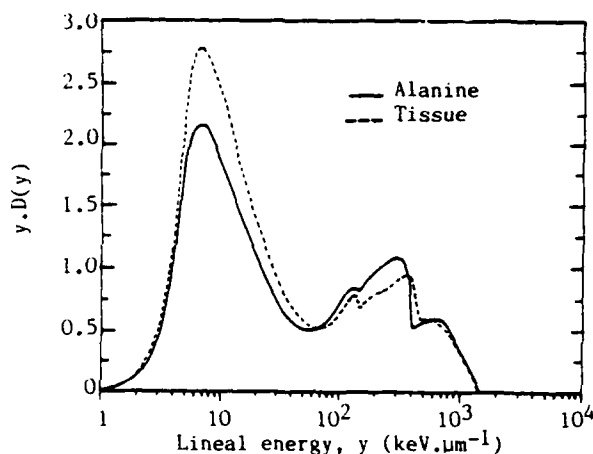

Figure 4. Same as Figure 3 except at a monoenergetic neutron energy of 16.9 MeV. Note that the large peaks have now shifted to a lower lineal energy; this is explained in the text.

Table 1. Elemental composition of alanine and tissue.

Material	H	C	N	O
Alanine	7.92	40.44	15.72	35.92
Tissue	10.20	12.30	3.50	74.00*

* In tissue, the six elements with a Z greater than 8 were considered to be oxygen. The per cent by weight of these few elements was equal to 1.10 and was added to that of oxygen.

Figures 5 and 6 show dose distributions as a function of lineal energy for alanine at neutron energies 1.1 and 16.9 MeV, respectively. The dashed curves show spectra of energy deposited by the charged particles weighted with the differential RE of the ions and normalised to the average RE for that neutron energy. This weighting and normalisation produces some distortion of the y spectra which can be seen by comparing the unmodified y spectra with the modified y spectra shown as solid curves in these figures. For example, for the 1.1 MeV neutrons, the proton edge — normally around 150 keV.μm^{-1} — is reduced to 90 keV.μm^{-1} because, in this region, the protons have a differential response which is lower than the average response for the 1.1 MeV neutrons. The shift is in the opposite direction for the region around 30 keV.μm^{-1}: in this region the protons have an average differential response which is greater than the average response for the neutrons. Although difficult to interpret because more charged particles are involved, similar reasoning explains the distortion for the weighted y spectrum for 16.9 MeV neutrons. The solid curves, shown in these two figures for comparison with the dashed curves, are the same as the solid curves shown in Figures 3 and 4.
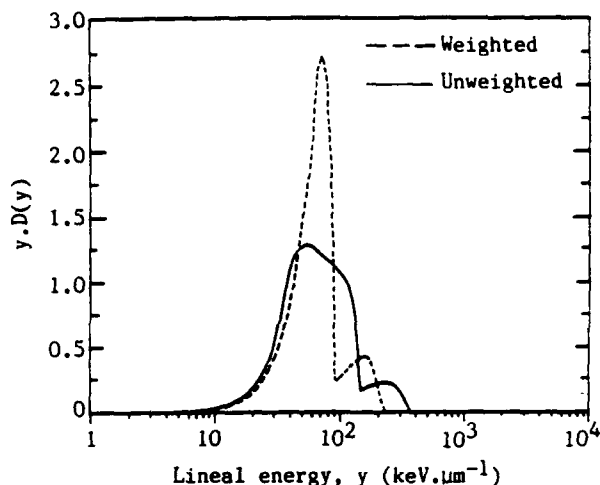
Figure 5. Calculated dose distributions in lineal energy for alanine determined at a neutron energy of 1.1 MeV. The dashed curve shows the spectrum of energy deposited by the charged particles weighted with the differential RE of the ions and normalised to the average RE for that neutron energy. This modification produces a distortion of the y spectrum which can be seen by comparing the modified spectrum with the unmodified spectrum shown as a solid line in this figure. The solid line is the unweighted distribution shown in the previous figure and repeated here for comparison with the weighted result. The reasons for the distortions are explained in the text.
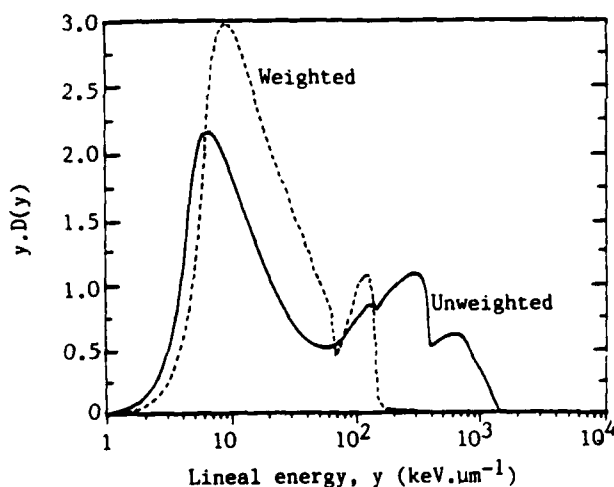

Figure 6. Same as Figure 5 except at a neutron energy of 16.9 MeV.

In general, the effect of the weighted RE on the dose distributions is the same for the results calculated at neutron energies 1.1 MeV and 16.9 MeV. Low y events are emphasised and high y events are de-emphasised because RE decreases with increasing LET. In addition, heavier ions also have a lower RE.

CONCLUSIONS

The RE for alanine has been calculated for monoenergetic neutrons with energies between 0.1 MeV and 17.1 MeV. Comparison of these results with measurements indicates general agreement but shows a somewhat higher calculated RE for lower neutron energies and a lower RE for higher neutron energies. The reason for these differences is being investigated.

The dose distribution as a function of lineal energy has been calculated at several neutron energies for alanine; comparison of these results is made with that of ICRU tissue. Differences observed are readily explained by the relative proportions of hydrogen, carbon, nitrogen, and oxygen found in the two materials.

Dose distributions for alanine, weighted with the differential RE values, were also calculated. The results when compared with the unweighted data show an increase of dose for low y events and a decrease of dose for the high y events. These results are consistent with a decreasing RE for values of high LET.

ACKNOWLEDGEMENTS

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